A HYBRID SAHA-EQUATION FOR RECOMBINING HIGH PRESSURE PLASMAS

IN WHICH Te ≥ Tg

by

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ABSTRACT

The question of steady state populations produced by a balance of heavy-particle collisional ionization against its inverse is considered. A hybrid-Saha approximation is derived which is useful in estimating the populations of excited states with high quantum numbers expected in plasmas recombining at high neutral pressures with an electron temperatures in excess of the heavy-particle temperature.

INTRODUCTION

Recently Bates and Khare[1] discussed a type of electron-ion recombination which could occur in high pressure plasmas in which the primary capture occurs according to the scheme

$$X^{+} + e + X \rightarrow X(\overset{*}{p}) + X \ , \tag{1}$$

where $X^{*}(p)$ denotes the p^{th} excited state of the X atom. The recombination is considered to be stabilized by subsequent superelastic collisions with heavy particles

$$X^{*}(p) + X \rightarrow X^{*}(q) + X \qquad p > q \ , \tag{2}$$

as well as by spontaneous radiation. Subsequently Collins[2] suggested that such processes might be considerably more important in laboratory plasmas in the Torr pressure range than had been previously suspected. Further it was suggested that contributions to the X^{*} population from such a process could conceivably explain the serious discrepancies between the intensity of radiation from the X^{*} population observed in certain experiments and that predicted by the otherwise successful theory of collisional-radiative recombination.[3] Although the method used by Bates and Khare to calculate the recombination rates neither depended on nor yielded excited state populations one can immediately infer that in the limit of high quantum numbers the excited state populations would be given by the Saha equation

$$N_n = N^+N_e \frac{g_n}{g^+g_e} \left(\frac{h^2}{2\pi mKTg}\right)^{3/2} \ell^{U_n/KT_g}, \qquad (3)$$

where: N_n, N^+, and N_e are the populations of the n^{th} bound level, ion, and free electrons, respectively, g_n, g^+, and g_e are the degeneracies of the n^{th} bound level, ion, and free electron, respectively, U_n is the ionization potential of the n^{th} bound level, T_g is the heavy particle temperature, m is the electron mass and other symbols have conventional meanings.

However, in many cases of possible interest such as early afterglows or active discharges the experimental plasma is non-thermalized, the electrons possessing a somewhat higher temperature than that of the heavy particles. This paper concerns the calculation of the excited state populations for recombination of the Bates-Khare type in the limiting case of a balance between collision-induced ionization and recombination i.e.

$$\frac{d[e]}{dt} = 0, \qquad (4)$$

but without the restriction that the electron temperature equal the gas temperature. Such a limiting case should provide an accurate approximation to excited state population in high pressure recombining plasmas for sufficiently high quantum numbers.

MATHEMATICAL METHOD

In the course of the calculations only recombination and ionization corresponding to (1) and its inverse were considered. In this case, referring to Figure 1 for identification of the energies involved, the ionization rate from the n^{th} bound level of X* to the differential level located in the continuum between E and E + dE can be written

$$dR_i = N_n dE \int_{\Delta}^{\infty} V_{rel}\, \sigma_{ex}\, (\Delta,e)\, dN(e), \qquad (5)$$

where N_n represents the population of the n^{th} bound level, V_{rel} the relative velocity between X and X*, σ_{ex} (Δ,e) the cross section per unit energy for transfer of energy between Δ and Δ+dE to X* from an X atom having kinetic energy of e/2 relative to the center of mass of X* and X, and dN(e) represents the distribution function for X as a function of e. Similarly the recombination rate from the differential state between E and E+dE into the n^{th} bound state of X* can be written

$$dR_R = \frac{dN(E)}{dE}\, dE \int_{0}^{\infty} V_{rel}\, \sigma_s\, (\Delta,e)\, dN(e), \qquad (6)$$

where now $\sigma_s(\Delta,e)$ is the cross section for the transfer of energy Δ from the $(X^+ + e)$ differential state to an X atom having kinetic energy of e/2 relative to the center of mass of X^+ and X, V_{rel} is the appropriate relative velocity, and $\frac{dN(E)}{dE}$ dE together represents the population of the differential state, N(E) being essentially the distribution function of free electrons.

In the absence of the restriction of equality of gas and electron temperatures we cannot require

$$dR_i = dR_R \tag{7}$$

for this would imply equilibrum among the free-free transitions at a temperature charisteristic of the heavy particle temperature. The weaker requirement

$$\int_{E=0}^{\infty} dRi = \int_{E=0}^{\infty} dR_R \tag{8}$$

is sufficient to produce a steady state balance between ionization from and recombination into to n^{th} bound level. Before substituting (5) and (6) into (8) it is expedient to evaluate several of the terms in (6). In particular the principle of detailed balancing[4.] serves to relate σ_s to σ_{ex} as follows:

$$\sigma_s(\Delta,e) = \sigma_{ex}\,(\Delta,\ e+\Delta)\ dE\ (1 + \frac{\Delta}{e})\ \frac{g_n}{dg(E)}\ , \tag{9}$$

where g_n is the statistical weight of the n^{th} bound level and dg(E) the statistical weight of the "continuum level" between E and E + dE.

This ratio is found from elementary quantum mechanics to be [5.6].

$$\frac{g_n}{dg(E)} = \frac{1}{2} N^{+} \frac{g_n}{g^{+} g_e} \left(\frac{E}{\pi}\right)^{1/2} \left(\frac{h^2}{2\pi m}\right)^{3/2} [dE]^{-1}, \tag{10}$$

where N^{+} is the X^{+} ion concentration, g_n, g^{+}, g_e are the statistical weights of the n^{th} bound state, X^{+} ion, and the free electron, and other constants have conventional meanings. Assuming the free electrons to be approximately described by the Maxwell-Boltzmann distribution characteristic of a higher electron temperature, Te, gives:

$$\frac{dN(E)}{dE} = \frac{2}{\pi} N_e \frac{E^{-1/2}}{(KT_e)^{3/2}} \ell^{-E/KT_e} . \tag{11}$$

Combining eq (9), (10) and (6) and substituting together with (5) into (8) gives:

$$N_n \int_0^\infty dE \left\{ \int_\Delta^\infty V_{rel} \sigma_{ex}(\Delta, e) dN(e) \right\} = N^{+} N_e \frac{g_n}{g^{+} g_e} \left(\frac{h^2}{2\pi m KT_e}\right)^{3/2} \int_0^\infty dE \left\{ \ell^{\frac{-E}{KT_e}} \int_0^\infty V_{rel} \sigma_{ex}(\Delta, e+\Delta)\left(1+\frac{\Delta}{e}\right) dN(e) \right\} . \tag{12}$$

Making the substitution on the right

$$e + \Delta = \varepsilon \ , \tag{13}$$

and further substituting a Maxwellian form for the distribution function of the X atoms gives with algebraic manipulation an implicit equation for the populations N_n as follows:

$$\int_0^\infty dE \left\{ \left[N_n - N^+ N_e \frac{g_n}{g^+ g_e} \left(\frac{h^2}{2\pi m K T_e}\right)^{3/2} \ell^{U_n/KT_g} \ \ell^{(1/KT_g - 1/KT_e)E} \right] \times \right.$$

$$\left. \int_{U_n+E}^\infty V_{rel} \cdot \sigma_{ex} (U_n + E, e) \ dN(e) \right\} = 0 \ , \tag{14}$$

where all terms are as previously identified and T_g represents the heavy particle temperature.

If a population decrement f_n is defined by the relation

$$N_n = N^+ N_e \frac{g_n}{g^+ g_e} \left(\frac{h^2}{2\pi m K T_e}\right)^{3/2} \ell^{U_n/KT_g} f_n \ , \tag{15}$$

then (14) can be simplified to give f_n in terms of the excitation cross sections σ as follows:

$$f_n = \int_{U_n}^\infty \ell^{\alpha(\Delta - U_n)} K(U_n, \Delta) d\Delta \left[\int_{U_n}^\infty K(U_n, \Delta) d\Delta \right]^{-1} \ , \tag{16}$$

where

$$\alpha = \left(\frac{1}{KT_g} - \frac{1}{KT_e}\right) , \qquad (17)$$

and $K(U_n,\Delta)$ is the rate coefficient per unit energy for the ionization of the n^{th} level with the emission of an electron of energy between E and E + dE, i.e.

$$K(U_n,\Delta) = \int_{\Delta}^{\infty} V_{rel}\, \sigma_{ex}\, (\Delta,e)\, dN(e) \quad . \qquad (18)$$

RESULTS

To solve for f_n exactly requires detailed knowledge, which is generally unavailable, of the ionization rate coefficient as a function of the ejected electron energy for the inverse of the process described in eq. (1). Classically, however, one would expect the difficulty of transferring large amounts of heavy particle energy, e, to the ejected electron would require $K(U_n,\Delta)$ to be a rapidly decreasing function of E. Further since $K(U_n,\Delta)$ is not a function of T_e, for a particular quantum level, n, an electron temperature, T_{max}, sufficiently close to T_g can always be found such that $\ell^{\alpha(E-U_n)} = 1$ over the range of E for which $K(U_n,\Delta)$ contributes significantly to the integrals in (16). Consequently for this particular n and electron temperature less than T_{max}, f_n is approximately unity and the excited state population is given by eq. (15) with $f_n = 1$.

The question now remains as to whether or not T_{max} is sufficiently larger than T_g to permit the simplified form of (15) with $f_n = 1$ to be used in the description of real plasmas of interest.

Figure 2 compares the results of substituting into eq. (15) the approximation $f_n = 1$ with the explicit calculations of f_n using the classical ionization rate coefficients $K(U_n,\Delta)$, given by Bates and Khare for helium. In the particular case presented $T_g = 300°K$ and the electron temperature is 1200°K. Lower electron temperatures were found to give even better agreement while higher electron temperatures gave agreement almost as good as would be expected from the fact that at a gas temperature of 300°K, α varies from zero to 38.7 ev^{-1} as T_e varies from 300°K to infinity, whereas the example presented for Te = 1200°K corresponds to an α of 29.0 ev^{-1}. Higher values of gas temperature were examined up to T_g = 1000°K and agreement was found to improve with increasing T_g in all cases in which $T_e > T_g$.

CONCLUSIONS

Although little experimental evidence is available on the detailed form of the ionization rate coefficient, $K(U_i,\Delta)$, as a function of the ejected electron energy, E; under the not particularly restrictive conditions discussed above it appears that the hybrid-Saha equation

$$N_n = N^+N_e \frac{g_n}{g^+g_e} \left(\frac{h^2}{2\pi mKT_e}\right)^{3/2} \ell^{U_n/KT_g} \tag{19}$$

is an approximation, sufficiently accurate for most purposes, of the excited state populations produced by an equilibrium between process (1) and its inverse under conditions in which the electron temperature is greater than the gas temperature.

REFERENCES

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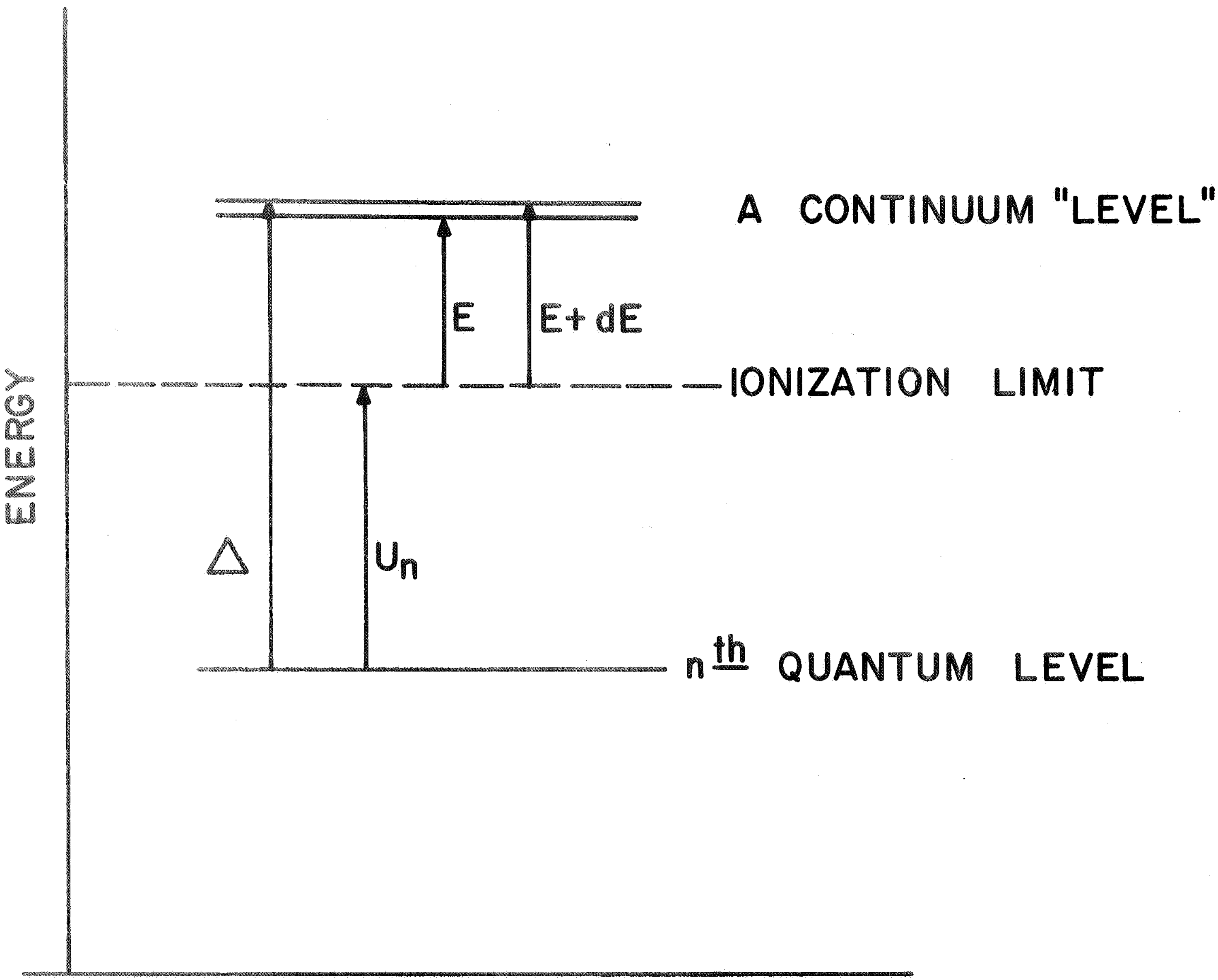
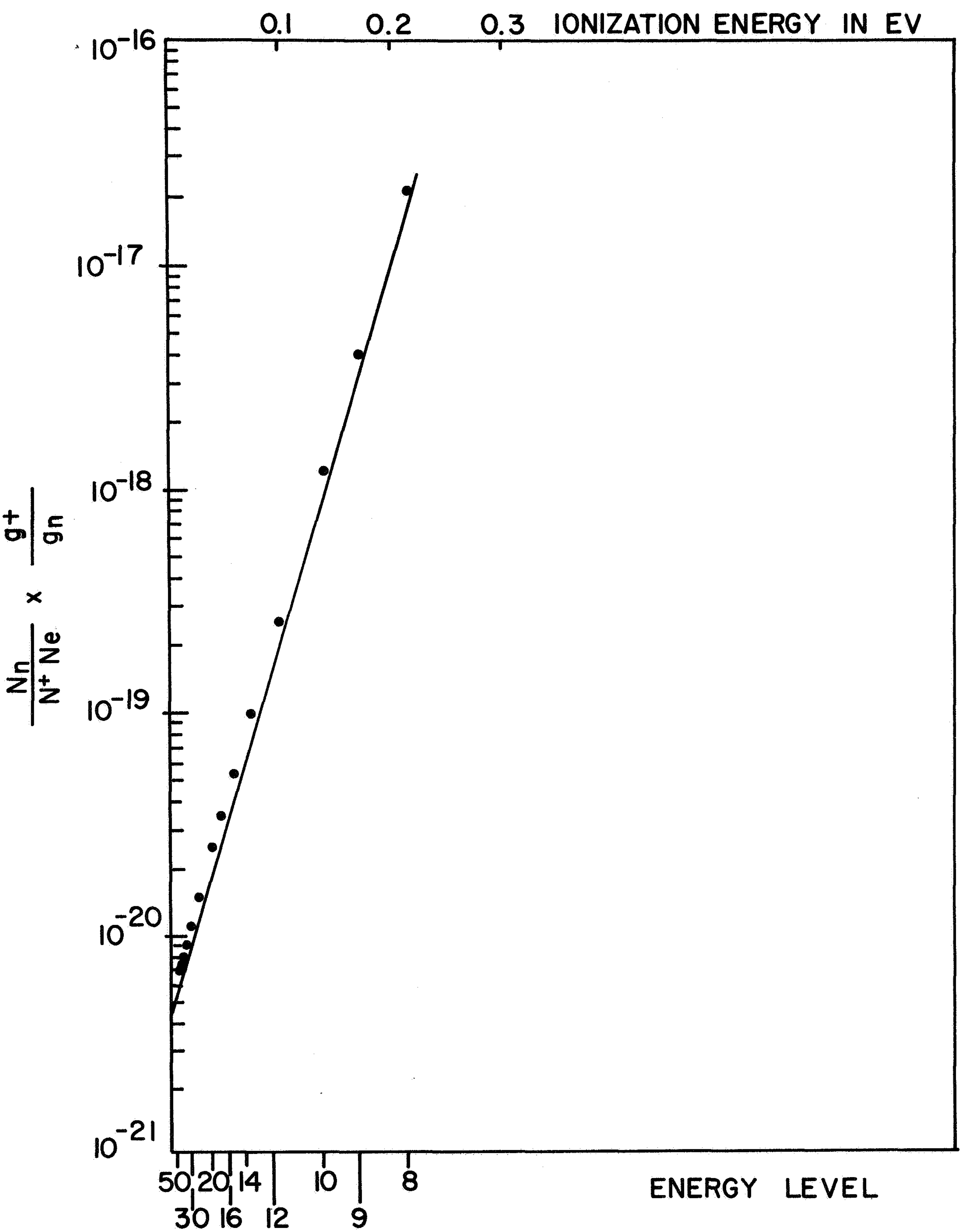
CAPTIONS

Figure 1: Schematic representation of the variables Δ, U_n, E, and dE appearing in text.

Figure 2: A graph of rationalized population per state of excited helium levels as a function of principal quantum number and ionization energy. The solid curve represents values obtained from the hybrid-Saha approximation, eq. (19). Points represent values obtained from eq (15) showing the results of including the explicit value of f_n.
$T_g = 300°K$, $T_e = 1200°K$



A CONTINUUM "LEVEL"
E
E + dE
IONIZATION LIMIT
ENERGY
Δ
U_n
n^{th} QUANTUM LEVEL



0.1
0.2
0.3
IONIZATION ENERGY IN EV
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
10^{-21}
$\frac{N_n}{N^+ N_e} \times \frac{g_+}{g_n}$
50
20
14
10
8
30
16
12
9
ENERGY LEVEL